

Demonstration of a robust pseudogap in a three-dimensional correlated electronic system

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Abstract

We outline a partial-fractions decomposition method for determining the one-particle spectral function and single-particle density of states of a correlated electronic system on a finite lattice in the non self-consistent T-matrix approximation *to arbitrary numerical accuracy*, and demonstrate the application of these ideas to the attractive Hubbard model. We then demonstrate the effectiveness of a finite-size scaling ansatz which allows for the extraction of quantities of interest in the thermodynamic limit from this method. In this approximation, in one or two dimensions, for any finite lattice or in the thermodynamic limit, a pseudogap is present and its energy diverges as T_c is approached from above; this is an unphysical manifestation of using an approximation that predicts a spurious phase transition in one or two dimensions. However, in three dimensions one expects the transition predicted by this approximation to represent a true continuous phase transition, and in the thermodynamic limit any pseudogap predicted by this formulation will remain finite. We have applied our method to the attractive Hubbard model on a three-dimensional simple cubic lattice, and find, similar to previous work, that for intermediate coupling a prominent pseudogap is found in the single-particle density of states, and this gap persists over a large temperature range. In addition, we also show that for weak coupling (an on-site Hubbard energy equal to one quarter the bandwidth) a pseudogap is also present. The pseudogap energy at the transition temperature is almost a factor of three larger than the $T=0$ BCS gap for intermediate coupling, whereas for weak coupling the pseudogap and $T=0$ BCS gap energies are essentially equal. These results show that a pseudogap due to superconducting fluctuations occurs in three dimensions even in the weak-coupling limit.

Keywords: Correlated electrons – theory, Hubbard model, spectral functions

I. INTRODUCTION

The theory of Bardeen, Cooper, and Schrieffer (BCS)¹ has been very successful in explaining a wide variety of phenomena associated with superconductivity. This is all the more remarkable since it is based on the independent quasi-particle approximation. Since very early on corrections to this simple picture have been investigated to explore what effect, if any, the breakdown of the quasi-particle approximation would have on various superconducting properties. One body of work in this category is the investigation of collective excitations, beginning with Anderson,² Bogoliubov *et al.*³, Rickayzen⁴ and others.⁵ Much of this work was directed towards a proper gauge-invariant description of the Meissner effect.

A separate line of work started with Migdal⁶ and Eliashberg,⁷ and investigated how the coupling of electrons to dynamical phonons would affect the quasiparticle properties of the electrons, including the transition temperature.

While this and other work⁸ focussed on properties in the superconducting state, a different line of enquiry concerned pairing fluctuations above T_c , as these could possibly cause deviations from the mean field picture provided by Fermi Liquid/BCS theory. Within BCS theory superconductivity arises through the formation of an order parameter, which has both an amplitude and a phase.⁹ Fluctuations can impact both the amplitude and the phase. At the present time phase fluctuations have been suggested to be relevant to the high- T_c problem. In particular, a school of thought^{10,11,12,13} suggests that electrons have a pair amplitude already above T_c , i.e. they exist as ‘pre-formed’ pairs. The superconducting transition is then simply the temperature at which the pairs acquire a common phase.¹⁴ The extreme case of this scenario is where two electrons already form a well-defined boson at the critical (i.e. phase-forming) temperature; this temperature is then the Bose condensation temperature for the system. A comprehensive review of such ideas has been provided by Randeria.¹⁵

These so-called pairing fluctuations would generally lead to a non-zero amplitude for pairing above T_c , with long-ranged superconducting order destroyed by fluctuations. One school of thought (to which we subscribe) suggests that some of the anomalous normal state properties observed in the high T_c systems, in particular the pseudogap, are due to pairing fluctuations, and a goal in this paper is the examination of such fluctuations in different dimensionalities using one particular controlled approximation scheme.

Specifically, one technical framework with which one can hope to understand this physics

is the so-called T-matrix approach. Within such a scheme, a pairing susceptibility can be defined;¹⁶ in the usual case,¹⁷ this pairing susceptibility diverges at T_c , the latter defined by BCS theory. Finding this temperature constitutes an alternate means of defining the transition temperature, and is generally known as the Thouless criterion.¹⁸ However, the existence of a diverging susceptibility (as one approaches the BCS critical temperature from above) should impact the single electron properties that determine the critical temperature in the first place. The T-matrix approximation accomplishes this through a renormalization of the potential an electron experiences. However, a limitation of this approach is that it can only be justified as a low density expansion of the two-particle Green's function.^{19,20}

Several many-body frameworks within which the T-matrix approximation can be cast have been discussed by Baym and Kadanoff and coworkers^{21,22,23} many years ago. The particular choice of framework unfortunately influences the results one obtains when calculations for a particular model system are actually performed. For example, in Ref.,²¹ a particular prescription for the single electron self-energy is derived through an equation-of-motion method. The resulting expression requires the use of two ‘levels’ of single electron Green functions, one bare, the other renormalized; that is, the latter contains a self-energy, and, consequently, such calculations must proceed self-consistently. Nonetheless, already in this work²¹ (see footnote 13 and the discussion at the end of section 3) it was recognized that certain features of this approximation were not acceptable.

Several years later the issue was debated some more,^{24,25,26} until what one could refer to as the ‘Patton fix’ emerged as the allegedly correct way to handle the difficulties with the Kadanoff-Martin prescription. In this adjustment, one of the self-consistent single electron Green functions is simply replaced with its non-self-consistent bare counterpart. This corrects some problems, but the adjustment is completely *ad hoc*, and has been called “non ϕ derivable”.²⁷ Such an approach has been championed recently by Levin and coworkers,²⁸ and has found some agreement with experiments on the high T_c cuprates.

Earlier, Baym²³ had formulated a theory of single electron and two particle properties based on functional derivatives of a free energy functional, a procedure which guaranteed that certain conservation laws would be satisfied. This formulation is known as a conserving approximation, and its extension to lattice electrons is known as the FLuctuation EXchange approXimation (FLEX)²⁹. When only the particle-particle channel is retained, the FLEX becomes a T-matrix theory with fully self-consistent single electron Green functions. Such

a formulation would appear to be the most accurate of the T-matrix approximations, since it includes the most number of diagrams. However, this claim is, in our opinion, unfounded. The possibility that vertex approximations (omitted in all T-matrix theories discussed here) partially cancel some of the self-energy contributions retained in the more fully self-consistent T-matrix approximations appears likely.³⁰ That is, including more channels and making everything self-consistent is not the panacea it might seem to be — this point has been emphasized in the alternative formulation of this problem by Vilk and Tremblay.³¹

It is probably fair to say that ‘modern’ interest, and a viable theoretical approach, on the influence of pair fluctuations on the superconducting transition was initiated by Leggett.³² This was later followed by an important paper by Nozières and Schmitt-Rink,³³ wherein they solved for the zero temperature properties of an electron gas with attractive interactions, for all coupling strengths. They showed that the BCS approximation gave the correct limiting behaviour in the strong coupling limit, where, in the lattice model at least, it was clear that the model was best described by tightly bound pairs of electrons. In this limit, it became clear that the superconducting transition was properly described by a Bose condensation of electron pairs. An important technical point raised in these two papers was that both the BCS gap equation and number equation were required, and had to be solved self-consistently.

This work was further extended to two dimensions in the context of the high T_c cuprates, by Schmitt-Rink, Varma, and Ruckenstein, in Ref.³⁴ They made the point that, for a specific (and fixed) electron density, as the temperature was lowered the chemical potential would self-consistently adjust so as to avoid the Thouless instability. (Note the necessity of adhering to the lesson from Ref.,³² that being that one must solve both for the normal state properties and the electronic density simultaneously.) In fact, all electron densities would result in a situation at $T = 0$ in which the Fermi surface no longer exists; the electrons are paired in bose-like bound states, and the chemical potential is simply half of the single pair bound state energy. This result violates Luttinger’s theorem.³⁵ Improvements were made by Serene,³⁶ Tokumitsu *et al.*³⁷, and later, for lattice fermions, by three of the present authors,³⁸ but the physics obtained in Ref.³⁴ remains. In fact, for lattice fermions the results are more physical, as the Thouless curve becomes a locus of points in the $T - \mu$ plane on which the electron density is identically equal to unity³⁸ (as opposed to a diverging quantity). Again, the simultaneous solution of the superconducting transition and the equation for the electronic density is required.

Since then a significant number of calculations have appeared on the T-matrix problems; see, for example, Refs.^{39,40,41,42,43,44,45,46,47} In addition, arguments against such formulations and in favour of alternate frameworks requiring vertex corrections, have also appeared.^{31,48,49,50} This body of work represents a significant advance in the study of the effect of fluctuations at temperatures above the superconducting transition. However, much of the ‘mathematical contortions’ that are invoked can be traced to the difficulty of studying two-dimensional systems in which the Mermin-Wagner theorem precludes the existence of true long-ranged order (in the systems studied here).⁵¹ Self consistency, and other formulations, aim to recover this result from any Thouless criterion approach (by which we imply theory attempting to identify T_c through a diverging pair susceptibility).

A simple remedy to avoid the Mermin-Wagner theorem is to study a three dimensional system. Therefore, in this paper we focus on a purely electronic Hamiltonian that yields a nonzero superconducting transition temperature, the attractive Hubbard model for a simple cubic lattice. Further, in three dimensions we can avoid the necessity of using a self-consistent theory, especially for weak coupling, and this is a simplification which will allow for us to solve for the self energy of a finite lattice, using the method outlined in the following sections of this paper, to essentially any numerical accuracy that we require.

In the above-described work, the appearance of a pseudogap, an experimentally observed phenomenon in which the single-particle density of states is suppressed in the form of an incompletely formed superconducting gap,⁵² is predicted. The literature on this question is now substantial — for a review of recent ideas see, for example, Ref.²⁷. A recurring theme in some of this work (see, *e.g.* Ref.⁵⁰) is that the pseudogap found in the high T_c cuprates can be associated with the two dimensional nature of the CuO planes. In terms of fluctuations, and in its simplest form, this is simply the statement that one expects enhanced fluctuations, towards the low-temperature phase, the lower the effective dimensionality of the system. The analysis that we present in this paper suggests that two dimensions may, in fact, not be necessary, because a pseudogap is found in the three dimensional attractive Hubbard model at weak coupling. For example, even at a temperature of a few per cent above the superconducting transition, in the three-dimensional attractive Hubbard model at half filling, clear evidence of a single-particle density of states pseudogap is found, and the magnitude of the gap is comparable to the BCS gap that would be found at $T = 0$.

We note that the number of papers on the 3d pseudogap is very small, compared to that

for the 2d problem, so comparisons with other work are difficult. Instead, here we shall simply address the question, should one expect a pseudogap in the 3d system with purely electronic attractive interactions?

II. FORMULATION

A. Model

We consider lattice fermions and the attractive Hubbard model; we restrict our attention to a kinetic energy that includes nearest neighbour hopping only. Working in the grand canonical ensemble thus leads us to consider the so-called Grand Hamiltonian \mathcal{K} defined by

$$\mathcal{K} = -t \sum_{\substack{\langle \mathbf{m}, \mathbf{m}' \rangle \\ \sigma}} (c_{\mathbf{m}\sigma}^\dagger c_{\mathbf{m}'\sigma} + c_{\mathbf{m}'\sigma}^\dagger c_{\mathbf{m}\sigma}) - \mu \sum_{\mathbf{m}, \sigma} n_{\mathbf{m}\sigma} - |U| \sum_{\mathbf{m}} n_{\mathbf{m}\uparrow} n_{\mathbf{m}\downarrow} . \quad (1)$$

In this equation t is the single particle hopping matrix element for nearest neighbour sites, μ is the chemical potential, $|U|$ is the on-site attractive potential, \mathbf{m} and \mathbf{m}' label the lattice sites, while $\langle \mathbf{m}, \mathbf{m}' \rangle$ denotes nearest neighbour sites (which are counted only once in the kinetic energy sum), and σ is the electron spin. The electron creation (annihilation) and number operators with spin σ at lattice site \mathbf{m} are given by $c_{\mathbf{m}\sigma}^\dagger$ ($c_{\mathbf{m}\sigma}$) and $n_{\mathbf{m}\sigma}$, respectively. We restrict ourselves to one-dimensional chains, and three-dimensional simple cubic lattices, and employ periodic boundary conditions.

B. One and Two Particle Propagators

Firstly, we define the required thermal Green's functions. The single electron Green's function⁵³ monitors the history of an electron injected at (imaginary) time τ'_1 and lattice site \mathbf{m}'_1 , and removed at time τ_1 and site \mathbf{m}_1 , and is defined by

$$G_\uparrow(\mathbf{m}_1, \tau_1; \mathbf{m}'_1, \tau'_1) = (-) \langle T_\tau [c_{\mathbf{m}_1\uparrow}(\tau_1) c_{\mathbf{m}'_1\uparrow}^\dagger(\tau'_1)] \rangle \equiv G_\uparrow(11') \equiv G(1-1') . \quad (2)$$

We use standard abbreviating notation, $1 \equiv (\mathbf{m}_1, \tau_1)$, and note that the last result of Eq. (2) follows from the translational periodicity, the time invariance, and spin isotropy of our lattice and Hamiltonian. Similarly, the two-electron propagator is given by

$$\begin{aligned} \mathcal{G}_{\uparrow\downarrow}(\mathbf{m}_1, \tau_1; \mathbf{m}_2, \tau_2; \mathbf{m}'_1, \tau'_1; \mathbf{m}'_2, \tau'_2) &\equiv \mathcal{G}(12; 1'2') \\ &= \langle T_\tau [c_{\mathbf{m}_1\uparrow}(\tau_1) c_{\mathbf{m}_2\downarrow}(\tau_2) c_{\mathbf{m}'_2\downarrow}^\dagger(\tau'_2) c_{\mathbf{m}'_1\uparrow}^\dagger(\tau'_1)] \rangle . \end{aligned} \quad (3)$$

(In this paper we will need to only consider the $\mathcal{G}_{\uparrow\downarrow}$ function, *viz.* the singlet channel, and thus spin indices of \mathcal{G} will not be shown.) This latter function's transform in momentum/energy space can be simplified by incorporating translational periodicity and temporal invariance, and we introduce the notation $Q \equiv (\mathbf{Q}, i\nu_Q)$ and $Q1 = \mathbf{Q} \cdot \mathbf{m}_1 + i\nu_Q\tau_1$. Then we have

$$\mathcal{G}(12; 1'2') = \frac{1}{(\beta N)^3} \sum_{Qqq'} e^{i\frac{Q}{2}((1+2)-(1'+2'))} e^{iq(1-2)} e^{iq'(1'-2')} \mathcal{G}(Q; qq') \quad (4)$$

where N is the number of lattice sites, Q is the centre-of-mass generalized momentum of either the outgoing or incoming pair, and q (q') is the relative momentum of the outgoing (incoming) pair of electrons, respectively. All wavevector summations span the first Brillouin zone, and Matsubara sums go over all integers.

From this function we extract the quantity that is our principal concern, *viz.* the pair propagator \mathcal{G}^{pair} which can be included in this set of equations in the following two ways:

$$\mathcal{G}^{pair}(Q) = \frac{1}{(\beta N)^2} \sum_{qq'} \mathcal{G}(Q; qq') \quad (5)$$

$$\mathcal{G}(11^+; 1'1'^+) = \frac{1}{(\beta N)} \sum_Q e^{iQ(1-1')} \mathcal{G}^{pair}(Q) . \quad (6)$$

An examination of Eqs. (4-6) shows that the pair propagator is equal to the probability of adding a pair of (opposite spin) electrons with one particular centre-of-mass momentum Q to *one* point in space, and then removing them as a pair at some other point in space (the centre-of-mass momentum Q is conserved at all collisions that occur between these points in time, and one must sum over all possible relative momenta, q and q').

The pair propagator's connection to superconductivity can be made apparent by introducing the pair annihilation operator via

$$\Delta_{\mathbf{Q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} c_{\frac{\mathbf{Q}}{2}+\mathbf{q}\uparrow} c_{\frac{\mathbf{Q}}{2}-\mathbf{q}\downarrow} \quad (7)$$

and then noting, by Eq. (5), that the pair propagator can be expressed as

$$\mathcal{G}^{pair}(Q) = \int_0^\beta e^{i\nu_Q\tau} \langle T_\tau [\Delta_{\mathbf{Q}}(\tau) \Delta_{\mathbf{Q}}^\dagger(0)] \rangle d\tau . \quad (8)$$

This equation most clearly allows one to understand the association of the pair propagator with the so-called pair susceptibility.¹⁶

Finally, it is instructive to extrapolate these relations to real times — one sees that one other way to interpret the behaviour of the pair propagator is that its analytic continuation

from imaginary frequencies to the complex plane allows one to evaluate the retarded pair propagator, in real time. As the discussion of Ambegaokar¹⁷ makes apparent, the poles of the pair propagator correspond to the relaxation times of a pair described by the retarded Green's function (also see Ref.²¹). Most of the poles correspond to continuum states comprised simply of two single (quasi-) electron states. Two poles are exceptions; initially these occur on the real axis. However, at sufficiently low temperature these poles form conjugate pairs on the imaginary axis. One of these poles signals an exponentially unstable (*viz.* growing) paired state implying that the normal state has now become unstable with respect to some new state whose stability is presumably related to these paired electrons. It is clear that, using this approach, one cannot proceed to temperatures below the critical temperature T_c . On the other hand, studying the pair propagator above this critical temperature is an ideal way to study pair fluctuations, as well as other properties of the fully interacting normal state. This formalism for identifying T_c from above has come to be known as the Thouless criterion.¹⁸

C. Non Self-Consistent T-Matrix Approximation

The above discussion motivates the analysis of the pair propagator in the normal phase. In order to find this function for the AHM we need to invoke a number of approximations. To be specific, we employ the ladder approximation to the Bethe-Salpeter equation for the reduced vertex. The derivations associated with this approximation, which leads to the T-matrix approximation for the single-particle propagator, are well known. It has been shown that this approximation is justified (see, *e.g.*, Ref.²⁰) in the limit of vanishing electron (or hole) densities.

The physical content of this approximation can be made most apparent if we begin with the equation for the 2-particle Green's function expressed in terms of the effective 2-particle interaction, which is given by (again, suppressing spin indices and sums over these indices)

$$\begin{aligned} \mathcal{G}(Q; q, q') &= \beta N \delta(q - q') G^0\left(\frac{Q}{2} + q\right) G^0\left(\frac{Q}{2} - q\right) \\ &- G^0\left(\frac{Q}{2} + q\right) G^0\left(\frac{Q}{2} - q\right) \Gamma(Q; q, q') G^0\left(\frac{Q}{2} + q'\right) G^0\left(\frac{Q}{2} - q'\right) \end{aligned} \quad (9)$$

where G^0 is the noninteracting single-electron Green's function. The ladder sum for the

effective interaction of the AHM, in a non self-consistent (NSC) calculation, is given by

$$\Gamma(Q; q, q') = -|U| + |U| \sum_k G^0(\frac{Q}{2} + k) G^0(\frac{Q}{2} - k) \Gamma(Q; k, q') . \quad (10)$$

This demonstrates that in the ladder approximation one includes scatterings of all orders in the particle-particle channel. Further, due to the independence of Γ on internal relative momenta, the solution of Eq. (10) is straightforward, *viz.*

$$\Gamma(Q) = \frac{-|U|}{1 - |U|\chi^0(Q)} \quad (11)$$

where the pair susceptibility of the noninteracting system is equal to

$$\chi^0(Q) = \frac{1}{N\beta} \sum_q G^0(\frac{Q}{2} + q) G^0(\frac{Q}{2} - q) . \quad (12)$$

Finally, using Eqs. (5,9,11) we can derive the pair propagator, or pair susceptibility $\chi(Q)$, in the NSC ladder approximation:

$$\mathcal{G}^{pair}(Q) = \chi(Q) = \frac{\chi^0(Q)}{1 - |U|\chi^0(Q)} \quad (13)$$

The solution of the Thouless criterion for the AHM treated in the NSC ladder approximation is now clear. The lifetime of a newly introduced (singlet) pair of electrons with crystal momentum \mathbf{Q} will first diverge (on cooling) when $Im\chi^0(Q) = 0$ and $1 - |U|\chi^0(Q) = 0$. The analytical properties of the pair susceptibility dictate that this must occur for zero Matsubara frequency, namely the Thouless criterion reduces to

$$\chi^0(\mathbf{Q}, 0) = \frac{1}{|U|} . \quad (14)$$

Hereafter, the locus of points in the $T - \mu$ plane which satisfies Eq. (14) shall be referred to as the Thouless criterion curve. For the AHM it can be shown^{54,55} that on cooling the transition defined by Eq. (14) first occurs for $Q = 0$, and from now on we define T_c in this manner.

As detailed in the introduction, we are interested in gaining an understanding of the effects of ‘feedback’,⁵⁶ that is when the pair fluctuations that are included in the pair propagator are introduced into the description of the single-electron properties. To this end, we evaluate the proper self-energy in the (same) NSC T-matrix approximation, resulting in

$$\Sigma(k) = - \frac{|U|^2}{\beta N} \sum_Q \chi(Q) G^0(Q - k) . \quad (15)$$

(Note that throughout this report we ignore the Hartree term, which can be simply absorbed into the chemical potential.) From this quantity the fully interacting single-particle Green's function is found via Dyson's equation

$$G(k) = \frac{1}{\{G^0(k)\}^{-1} - \Sigma(k)} . \quad (16)$$

The important quantity in this paper, the single-particle density of states (DOS), is related to the one-electron spectral function, given by

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} G(\mathbf{k}, \omega + i0^+), \quad (17)$$

which leads to the DOS given by

$$\mathcal{N}(\omega) = \frac{2}{N} \sum_{\mathbf{k}} A(\mathbf{k}, \omega). \quad (18)$$

D. Partial Fractions Decomposition

The above equations are well known. Here we present an approach that allows for us to solve for all of the spectral functions of finite lattices in the above-described NSC T-matrix approximation to arbitrary numerical accuracy — in one dimension we can solve for chains of lengths up to 128 (which has 65 inequivalent \mathbf{k} points in the first Brillouin zone), while in three dimensions we have solved lattices up to a size of twelve cubed (which has 84 inequivalent \mathbf{k} points in the first Brillouin zone) — and to then extract information about the density of states in the thermodynamic limit. To complete the decomposition for a twelve cubed lattice at one temperature and chemical potential can take up to ten days on a high-speed 64-bit (which is essential) alpha processor; so, it is not a simple matter to obtain large sets of data using this approach.

To solve for the one-particle self energy we first note that the non-interacting pair susceptibility, defined in Eq. (12), can be written in terms of a sum over wave vectors

$$\chi^0(\mathbf{Q}, \nu_n) = \frac{1}{N} \sum_{\mathbf{k}} \frac{f[\xi_{\mathbf{k}}] + f[\xi_{\mathbf{Q}-\mathbf{k}}] - 1}{i\nu_n - \xi_{\mathbf{k}} - \xi_{\mathbf{Q}-\mathbf{k}}}, \quad (19)$$

where $f[\xi]$ represents the Fermi-Dirac distribution function at a temperature T and chemical potential μ , $\xi_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} - \mu$, and $\varepsilon_{\mathbf{k}}$ is the noninteracting band electron dispersion (*e.g.*, $\varepsilon_k = -2t \cos(k)$ in one dimension). The analytic continuation of this function to the complex

plane, denoted by $\chi \rightarrow \bar{\chi}$, is achieved trivially by the substitution $i\nu_n \rightarrow z$. Thus, from Eq. (13) we can write the pair propagator as

$$\bar{\chi}(\mathbf{Q}, z) = \frac{\bar{\chi}^0(\mathbf{Q}, z)}{1 - |U|\bar{\chi}^0(\mathbf{Q}, z)} = \frac{1/N \sum_{\mathbf{k}} \frac{f[\xi_{\mathbf{k}}] + f[\xi_{\mathbf{Q}-\mathbf{k}}] - 1}{z - \xi_{\mathbf{k}} - \xi_{\mathbf{Q}-\mathbf{k}}}}{1 - |U|/N \sum_{\mathbf{k}} \frac{f[\xi_{\mathbf{k}}] + f[\xi_{\mathbf{Q}-\mathbf{k}}] - 1}{z - \xi_{\mathbf{k}} - \xi_{\mathbf{Q}-\mathbf{k}}}}. \quad (20)$$

If one simply expands the wave vector sums, it is seen that this function admits a partial fraction decomposition. Incorporating the requisite analytical properties of this 2-particle propagator (the chosen signs follow from the spectral representation of the 2-particle GF) we choose to write this expansion as

$$\bar{\chi}(\mathbf{Q}, z) = -\frac{\text{sgn}(E_{\mathbf{Q}}^{(1)})R_{\mathbf{Q}}^{(1)}}{z - E_{\mathbf{Q}}^{(1)}} - \frac{\text{sgn}(E_{\mathbf{Q}}^{(2)})R_{\mathbf{Q}}^{(2)}}{z - E_{\mathbf{Q}}^{(2)}} - \dots \quad (21)$$

where the number of poles for each \mathbf{Q} is denoted by $s_{\mathbf{Q}}$, the energies $E_{\mathbf{Q}}^{(\ell)}$ are real, and the residues $R_{\mathbf{Q}}^{(\ell)}$ are strictly positive, for $\ell = 1, \dots, s_{\mathbf{Q}}$. Substituting this into Eq. (15) and completing the Matsubara frequency sum analytically allows us to restate the expression for the self energy in the convenient form

$$\bar{\Sigma}(\mathbf{k}, z) = \frac{U^2}{N} \sum_{\mathbf{Q}} \sum_{l=1}^{s_{\mathbf{Q}}} \frac{\text{sgn}(E_{\mathbf{Q}}^{(l)})R_{\mathbf{Q}}^{(l)}(f[\xi_{\mathbf{Q}-\mathbf{k}}] + b[E_{\mathbf{Q}}^{(l)}])}{z + \xi_{\mathbf{Q}-\mathbf{k}} - E_{\mathbf{Q}}^{(l)}}, \quad (22)$$

where $b[E]$ is the Bose-Einstein distribution for temperature T with the chemical potential set equal to zero.

The application of the above results requires the determination of the poles and residues of the partial fraction expansion of the pair propagator. This is a complicated task, and we have completed our calculations using a computer algebra system allowing for a symbolic calculation that produces numerical results for the poles and residues.⁵⁷ Also, note that the result of this partial-fractions formulation is a DOS that is a series of delta functions – we have broadened each of the single-particle spectral peaks with Lorentzians with a fixed broadening of 3% of the bandwidth, namely $0.12t$ in one dimension, and $0.36t$ in three dimensions.

III. EXAMINATION OF THE 1D PSEUDOGAP - TEST CASE

As an example of the application of this method, we have examined one dimensional (1d) chains. We stress that this is not, and is not intended to be, a solution of the 1d AHM, which cannot be accomplished through the use of the T-matrix approximation. Instead we use these results as a means of demonstrating how our results can be applied, via a finite-size scaling extrapolation to the thermodynamic limit, to estimate the bulk value of the (pseudo)gap.

In Fig. 1 we show the DOS of a one-dimensional chain with periodic boundary conditions of varying lengths (16×1 up to 128×1) with $|U|/t = -2$ in the non self-consistent T-matrix approximation for the AHM. We have taken this data for a fixed (non-interacting) electronic density per lattice site of $\langle n \rangle = 0.5$, corresponding to $1/4$ filling. The temperature is fixed to be just above the BCS transition temperature, and to account for the fact that the BCS transition temperature depends on the length of the system, we have used a varying temperature of $1.001 T_c(L)$, thus corresponding to a fixed ratio of $T/T_c(L)$ for all system sizes.

It is clear from Fig. 1 that each DOS curve contains sharply peaked structures, and it is natural to associate the location of these peaks with something analogous to the superconducting gap. Of course, these data are evaluated in the normal phase, and the DOS does not ever go strictly to zero (near $\omega/t = 0$) in the normal phase, so the locations of the peaks are not true superconducting gaps, but can be thought of as something akin to (single-particle DOS) (pseudo)gaps.

These data display strong finite size effects, and the obvious question is, what does the DOS look like in the thermodynamic limit? We now demonstrate how one can answer this question, and thus use data such as that shown in Fig. 1 to correctly extrapolate to the thermodynamic limit. This analysis will lead us to a controlled manner of both verifying the existence of, and quantitatively estimating, the pseudogap in three dimensions.

The finite-size scaling corrections to the wave vector sums that are encountered in this problem go as

$$\frac{1}{L} \sum_q = \frac{1}{2\pi} \int_{-\pi}^{\pi} dq + \left(\frac{1}{L} \sum_q - \frac{1}{2\pi} \int_{-\pi}^{\pi} dq \right) \sim \frac{1}{2\pi} \int_{-\pi}^{\pi} dq + \mathcal{O}\left(\frac{1}{L^2}\right). \quad (23)$$

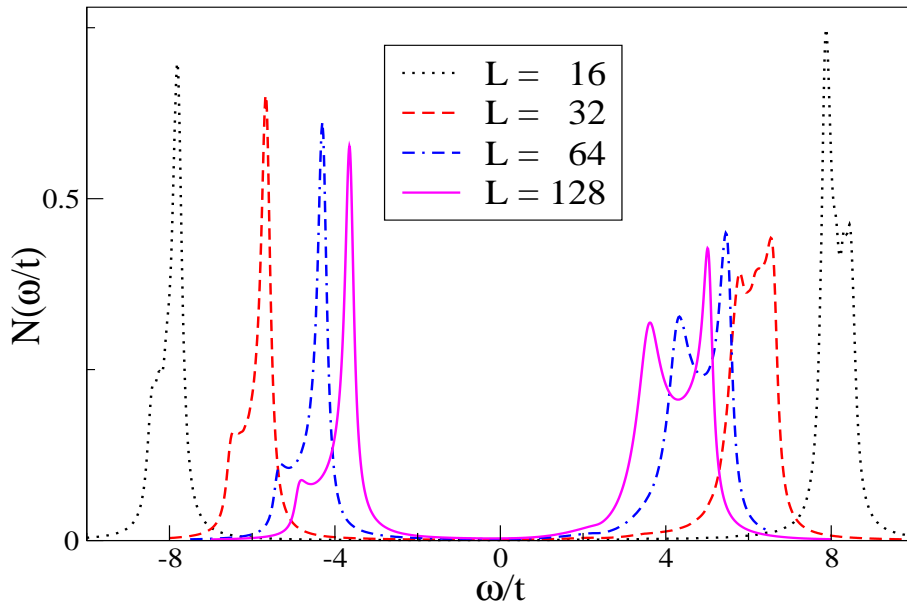


FIG. 1: The density of states (DOS) of the 1d attractive Hubbard model evaluated in the non self-consistent T-matrix approximation for 16×1 , 32×1 , 64×1 , and 128×1 chains with periodic boundary conditions, for $|U|/t = -2$ and a fixed (noninteracting) electronic density per lattice site of $\langle n \rangle = 0.5$, corresponding to $1/4$ filling; the temperature used for each curve is $1.001 T_c(L)$. Each delta-function peak of the spectral function has been broadened as a Lorentzian using a fixed broadening energy of 3 % of the bandwidth — through experimentation we have found that such a broadening produces smooth density of states curves without washing out important structure.

Thus, noting that the peak locations, which from now on are provocatively labelled as Δ , from Fig. 1 can be associated with a strong divergence of one particular contribution (see below) to the self energy, and that the wave vector sums in Eq. (15) should have the same finite-size scaling corrections as given in Eq. (23), we expect that the peak locations of, *e.g.*, Fig. 1, should approach their values in the thermodynamic limit as $\sim 1/L^2$. This is precisely the form that we find, as is shown in Fig. 2.

We now focus on the values of Δ obtained from using the above-shown finite scaling analysis extrapolated to the thermodynamic limit. To be specific, we now show that the divergence of this (pseudo)gap as T approaches T_c from above is precisely what should be found in the thermodynamic limit. This successful extraction of $\Delta(L \rightarrow \infty)$ helps to support our contention that such a finite-size scaling analysis is a reliable procedure for extracting

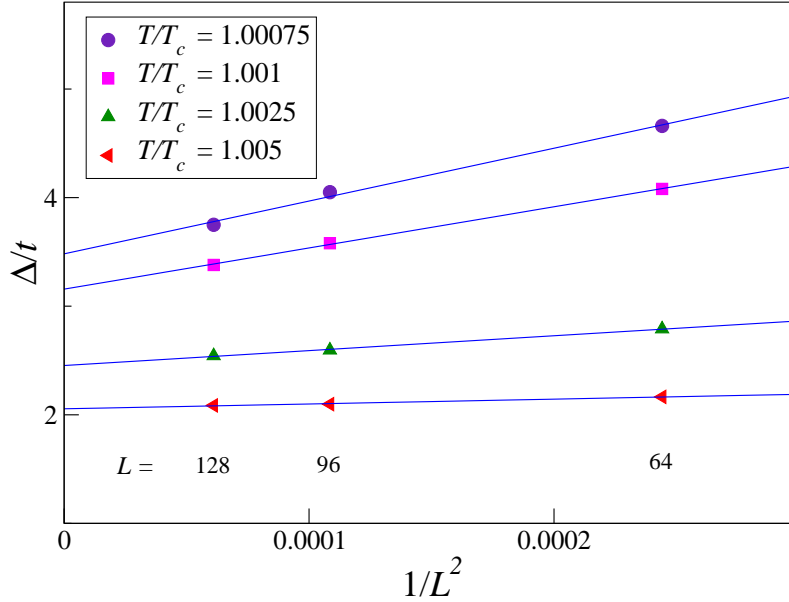


FIG. 2: The locations of the peaks, labelled as Δ and expressed in units of t , found in the 1d DOS (*e.g.*, see Fig. 1), plotted as a function of one over the the system's length (L) squared, for a variety of temperatures (shown in the legend) just above the superconducting transition temperature. The same parameters as in Fig. 1 are used. The solid lines are least squares fits to the data for each of these temperatures.

the bulk value of this energy.

To this end, we first require the behaviour of the self energy as the Thouless criterion is approached from above. It is instructive to return to the definition of the self energy (prior to making a partial fractions expansion) given in Eq. (15). All quantities in Eq. (15) are known exactly (although $\chi^0(\mathbf{q}, i\nu_n)$ requires a momentum sum – see Eq. (12)); nonetheless, it is not in a convenient form from which the DOS in the $L \rightarrow \infty$ limit can be extracted. That is, while one can successfully approximate the wave vector integration over the first Brillouin zone with discrete momentum sums (with a dense mesh of k points) for higher temperatures, such a method is doomed to fail for temperatures/chemical potentials near the Thouless curve. This is because the denominator in the kernel of Eq. (15) (*i.e.*, the denominator of Eq. (13)) approaches zero (for $\mathbf{q} = 0$ and $i\nu_n = 0$). To be specific, using a discrete momentum sum over the wavevectors of a finite lattice will result in a self energy that diverges as $T \rightarrow T_c$ in any dimension, for any finite lattice. However, phase space

arguments following the Mermin-Wagner theorem⁵⁸ show that the self energy in the form of Eq. (15) should **not** diverge in three dimensions – see below. Thus, we need to examine Eq. (15) more carefully to properly understand the distinction between one (and two) and three dimensions, and to properly extract the temperature dependence of the (pseudo)gap as T_c is approached from above.

Since the Thouless criterion arises from the $i\nu_n = 0$ term in the Matsubara frequency, it is prudent to treat the $n = 0$ part of the self energy sum separately. Then, to correctly deal with the $\mathbf{q} \rightarrow 0$ contribution, we have separated the $i\nu_n = 0$ term into two contributions — the one from $\mathbf{q} \neq 0$ is given by

$$\Sigma_{nzq}(\mathbf{k}, i\omega_m) = -|U|^2 \frac{1}{N\beta} \sum'_{\mathbf{q}} \chi(\mathbf{q}, 0) G^0(-\mathbf{k} + \mathbf{q}, -i\omega_m). \quad (24)$$

and the one from \mathbf{q} near zero is done by an integration (which is correct, and as we show necessary, if we completed the entire calculation in the thermodynamic limit),

$$\Sigma_{zq}(\mathbf{k}, i\omega_m) = -|U|^2 \frac{1}{\beta} \int_{-q_0}^{q_0} \frac{d^d q}{(2\pi)^d} \chi(\mathbf{q}, 0) \frac{1}{-i\omega_m - (\epsilon_{-\mathbf{k}+\mathbf{q}} - \mu)}, \quad (25)$$

where \mathbf{q}_0 represents an upper cutoff for the part of the first Brillouin zone in which we will integrate over the integrand analytically, and d represents the dimensionality of the space. The prime in the summation of Eq. (24) indicates that this same small \mathbf{q} region is omitted from Σ_{nzq} . Thus, in all expressions except the last (Eq. (25)) we will simply perform \mathbf{q} -sums over finite lattices (which amounts to the trapezoidal rule for numerical integration), while in the latter equation it is important to integrate analytically over the integrand.

To this end we require an explicit expression for $\chi^0(\mathbf{q}, 0)$, which is difficult to obtain. Instead, we approximate it with an expression valid for small \mathbf{q} :

$$\chi^0(\mathbf{q}, 0) \approx a^2 - b^2 q^2, \quad (26)$$

where $q = |\mathbf{q}|$ and a^2 and b^2 are obtained by fits to $\chi^0(\mathbf{q}, 0)$. In one dimension this is a simple matter of fitting the susceptibility at $q = 0$ and at some small $q = q_0$, and an example case is shown in Fig. 3; clearly, this is an excellent approximation for small q . Then, expanding the band dispersion $\epsilon_{-\mathbf{k}+\mathbf{q}}$ for small \mathbf{q} , the integral in Eq. (25) can be written as

$$\Sigma_{zq}(k, i\omega_m) \approx \frac{2|U|^2}{\pi\beta} \int_0^{q_0} dq \left(\frac{a^2 - b^2 q^2}{A + Bq^2} \right) \left(1 - \left[\frac{1}{2} \epsilon_k'' G^0(k, -i\omega_m) + (\epsilon_k')^2 (G^0(k, -i\omega_m))^2 \right] q^2 \right). \quad (27)$$

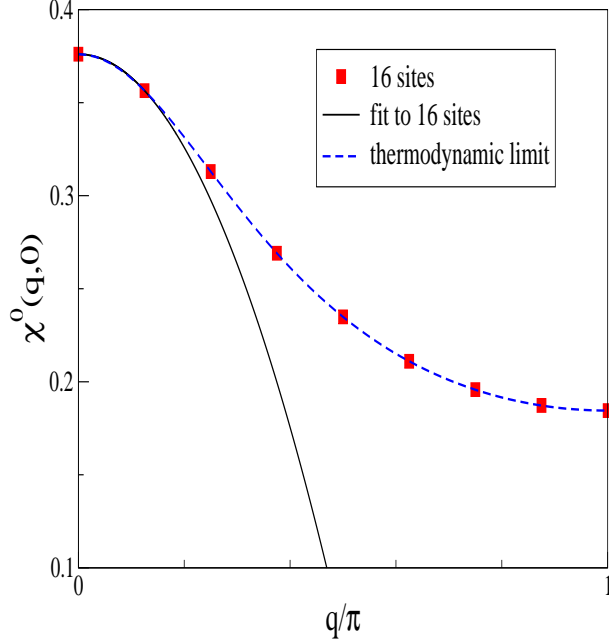


FIG. 3: Real part of the non-interacting susceptibility *vs.* q in one dimension. Red squares are for a 16 site lattice, while the green curve is based on the fit as described in the text. The blue curve is the result in the thermodynamic limit. Clearly, the black curve reproduces very accurately the thermodynamic limit result at low q , even though the green curve is obtained on the basis of a fit to the two lowest points ($q = 0$ and $q = \pi/8$).

We have introduced $A \equiv 1 - |U|a^2$ and $B = |U|b^2$, and note that both are positive numbers. Further, and most importantly, since $\chi^0(0, 0) \sim 1/T$ at low temperatures, we obtain that A is approaching zero linearly in T from above as $T \rightarrow T_c$. That is, $A \sim |\alpha|(T - T_c)$ for α being some constant. (This clarifies the “mean-field” label that can be applied to the non self-consistent T-matrix approximation.)

All of the integrals in this expression are elementary; the important contribution comes from

$$\int_0^{q_0} dq \left\{ \frac{1}{A + Bq^2} \right\} = \frac{1}{\sqrt{AB}} \tan^{-1} \left(q_0 \sqrt{B/A} \right), \quad (28)$$

which diverges as $1/\sqrt{T - T_c}$ near the Thouless curve. Since we have employed the (non self-consistent) T-matrix approximation, it is correct that this quantity diverges in 1d; however, had we not handled this integration analytically (and instead proceeded with lattice sums for a large but finite lattice) we would have obtained a divergence proportional to $1/(T - T_c)$ instead, which is incorrect in the thermodynamic limit.

The behaviour of the $L \rightarrow \infty$ (pseudo)gap Δ can now be identified through a (mean-field like) ansatz for the (pseudo)gap given by

$$\Sigma(k, i\omega_n) = \frac{\Delta^2}{i\omega_n + \xi_k} . \quad (29)$$

This ansatz has been proposed by various authors; Moreo *et al.*⁵⁹ remarked that the mean-field theory of Schrieffer *et al.*⁶⁰ predicts such a form. The TPSC theory of Vilk and Tremblay³¹ leads to the same functional form for estimating the magnitude of the pseudo-gap. Also, the work of the group of Levin²⁸ has produced and critiqued this ansatz. Lastly, we note that three of the present authors showed how such a form arises in a self-consistent T-matrix formulation.³⁸

We augment support for this ansatz by noting that when the (pseudo)gap parameter Δ is evaluated in the non self-consistent T-matrix approximation (in 1d), focussing on the $i\Omega_n$ term in the Matsubara frequency sum, which diverges at T_c , one expects that

$$\Delta^2 = \frac{|U|^2}{\beta L} \sum_q \frac{\chi^0(q, 0)}{1 - |U|\chi^0(q, 0)} . \quad (30)$$

Here we note the following successes of this ansatz: (I) Using the finite-size scaling result of Eq. (23), Eq. (30) predicts that $\Delta^2(L) = \Delta^2(L \rightarrow \infty) + \mathcal{O}(1/L^2)$, which also implies that a $1/L^2$ scaling should be found for Δ ; this is precisely the form that we find, as shown in Fig. 2. (II) If this ansatz is used to derive the DOS when the system is close to the Thouless criterion line for large L , good agreement is found. To be specific, if one solves for the temperature-dependent (pseudo)gap using Eq. (30), and then uses this value in Eq. (29), and then analytically continues to the real axis to find the spectral function $A(k, \omega)$ through Eq. (17), one finds

$$A(\mathbf{k}, \omega) = \frac{1}{2} \left(1 + \frac{\xi_{\vec{k}}}{\sqrt{\xi_k^2 + \Delta^2}} \right) \delta(\omega - \sqrt{\xi_k^2 + \Delta^2}) + \frac{1}{2} \left(1 - \frac{\xi_{\vec{k}}}{\sqrt{\xi_k^2 + \Delta^2}} \right) \delta(\omega + \sqrt{\xi_k^2 + \Delta^2}) . \quad (31)$$

Then, to facilitate a comparison with our partial fractions results, one must broaden the delta functions in Eq. (31) in an analogous manner to that used in our partial fractions decomposition, that is each delta function is replaced by a Lorentzian with a fixed broadening of $0.12t$. Finally, a direct comparison of the DOS from both the exact partial fractions expansion and the above described method yields very good agreement, in particular for the locations of the peaks closest to the “gapped region”. An example of such a comparison is

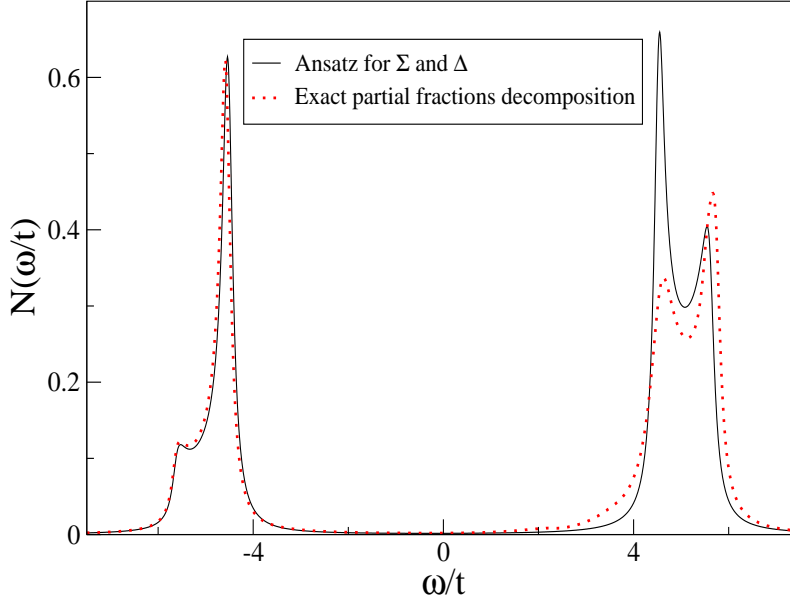


FIG. 4: A comparison of the “exact” DOS of a finite 1d system, calculated within the NSC T-matrix approximation, to that predicted by Eq. (29). The (pseudo)gap parameter Δ is found from Eq. (30), and then the density of states is calculated by using a wave vector sum of the spectral functions given in Eq. (31). For these calculations the system parameters are $L=128$, $U/t = -2$, $\langle n \rangle_0 = 0.5$, and $T/T_c(L) = 1.0005$, where a broadening of $0.12t$ has been used in both calculations.

shown in Fig. 4. This agreement is exceptional given the crude nature of the approximation in Eqs. (29,30).

Thus, from Eq. (28) one expects that Σ diverges as $1/(\sqrt{T - T_c})$, and then using Eq. (29) the (pseudo)gap should diverge as $1/(T - T_c)^{1/4}$ (in fact, this result can be directly extracted from Eq. (30)). This is precisely the temperature dependence that we find – in Fig. 5 we show the $L \rightarrow \infty$ extrapolated (pseudo)gap *vs.* the reduced temperature, defined by $\delta T = (T - T_c)/T_c$, fit to the form $1/\delta T^\kappa$, and obtain an exponent $\kappa = 0.27 \pm 0.03$.

Note that despite the potential difficulties of making a precise determination of the peak position (*e.g.*, accounting for systematic errors introduced through the use of some fixed constant Lorentzian broadened peaks obtained from the partial fractions decomposition), the obtained fit to the data is excellent, with a critical exponent very close to the expected value of $1/4$.

We note that one may complete similar calculations in two dimensions, and again the

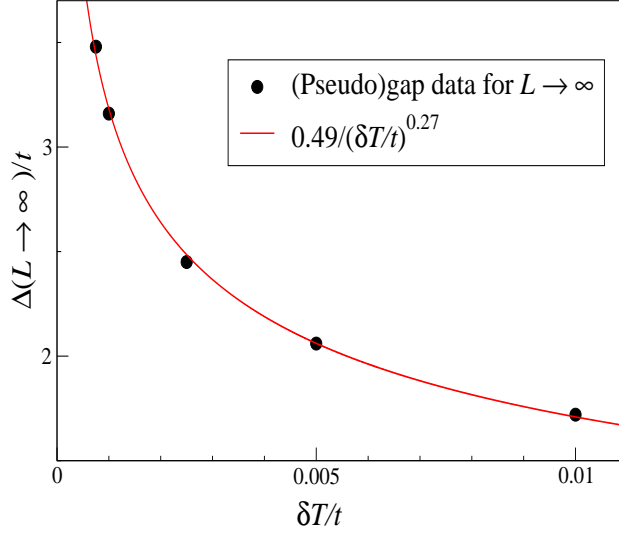


FIG. 5: The locations of the peaks, extrapolated to the thermodynamic limit using the previously described analysis, plotted as a function of the reduced temperature, defined by $\delta T = (T - T_c)/T_c$, just above the superconducting transition temperature. The same parameters as in Fig. 1 are used. The solid line shows the least-squares fit of the data to the functional form $\Delta/t \sim (\delta T)^\kappa$, where we find $\kappa = 0.27 \pm 0.03$.

(pseudo)gap energy diverges to infinity as the transition temperature is approached from above. However, in two dimensions this divergence is logarithmic, a result that follows from Eq. (25), and thus unless one is very close to the transition, this divergence is difficult to find. For example, the real-axis analysis of the T-matrix approximation in two dimensions of Metzner *et al.*⁴⁵ finds spectral functions and pseudogaps similar to what we find, but they did not go to small enough reduced temperatures to observe the (unphysical) diverging pseudogap. (What is needed to suppress this unphysical divergence, which can be traced to the unphysical divergence of the effective vertex, is a theory beyond the non self-consistent T-matrix approximation.^{31,38})

We believe that the sequence of calculations outlined above for one dimension, *viz.* (i) perform a partial fractions expansion of the pair propagator, thus obtaining the poles and residues of the one-particle Green's function (for a finite lattice) to arbitrary numerical accuracy, and (ii) extrapolating to the thermodynamic value of the (pseudo)gap as a function of the reduced temperature using Eq. (23), is justified, in part by the above demonstration.

IV. A PSEUDOGAP IN THREE DIMENSIONS

We now describe the result that is central to the goal and message of this paper, *viz.* a single-particle DOS pseudogap above the superconducting T_c can be present in three dimensions, even in the weak coupling limit.

To begin, we first note the qualitative change that arises from an analysis of the behaviour of the self energy in three *vs.* one (or two) dimensions. That is, according to Eq. (25), even when the denominator of $\chi(q, 0)$ vanishes at $q = 0$ the self energy remains finite. It is this difference that makes the study of the AHM on a three-dimensional lattice so attractive (no pun intended). That is, one correctly predicts a true phase transition at a nonzero temperature, and the Mermin-Wagner theorem does not disallow such a transition in three dimensions – it is the true superconducting phase transition that such a system will undergo.

We have repeated the analysis of the previous section for a three-dimensional simple cubic lattice with periodic boundary conditions. As system parameters we have used $|U|/t = 6$ and 3 (that is, $|U| = W/2$ and $|U| = W/4$, where $W = 12t$ is the noninteracting bandwidth in three dimensions). The first of these ratios is the same as the on-site attractive interaction energy to bandwidth that was used in the previous section's study of the 1d AHM, while the second is in the weak-coupling limit. Also, in part due to the interest in the cuprate superconductors and doped Mott insulators, we have examined a (noninteracting) electronic density of $\langle n \rangle_0 = 1$, *viz.* half filling.

Results for the DOS for different size lattices are shown in Fig. 6 for $|U|/t = 6$, for a reduced temperature of 0.0001. As in the previous section, we have broadened the delta functions that emerge from the partial fractions decomposition with a fixed energy equal to 3 % of the noninteracting bandwidth, which is $0.36t$ for the simple cubic lattice. It is to be emphasized that there are *no* true superconducting gaps in these spectra, in that the DOS is never reduced to zero at the Fermi level (which is located at $\omega = 0$).

How does the DOS develop as a function of the attractive Hubbard energy U ? In Fig. 7 we show the change of the DOS as $|U|/t$ is decreased from 6 to 3, using a reduced temperature of 0.001 for each value of $|U|$, for a 12^3 lattice; that is, $T/T_c(|U|, L) = 1.001$. As a reference curve, we also show the $U = 0$ noninteracting DOS in the thermodynamic limit.

The scaling of the peak positions, which we now label as Δ_{pg} , *vs.* system size is shown in Fig. 8, and we again find a finite-size scaling behaviour that clearly goes as $1/L^2$. From

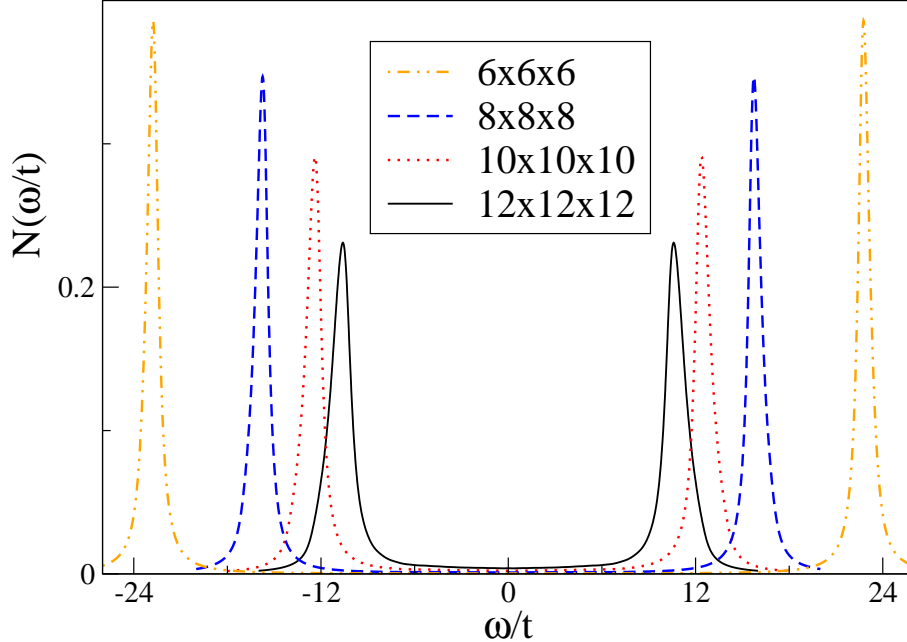


FIG. 6: The single-particle DOS for simple cubic lattices of size 6^3 , 8^3 , 10^3 , and 12^3 , for $|U|/t = 6$ and $1/2$ filling, at a temperature of $T/T_c(L) = 1.0001$. We have employed a fixed broadening of 3% of the noninteracting bandwidth, namely $0.36t$.

this figure one sees that all extrapolated values for small reduced temperatures are very close to one another (approximately $6.5t$ for these material parameters), and do not go to zero, or infinity, as the reduced temperature is lowered towards zero. Further, one can use BCS theory¹ to calculate the superconducting energy gap at $T = 0$, and for $1/2$ filling and $|U|/t = 6$ one finds a gap of about $2.3t$, roughly $1/3$ of the energy of the pseudogap found in Fig. 8 (which is evaluated just above T_c , and not $T = 0$!).

How does the pseudogap behave as a function of temperature? As seen in Fig. 8, for $\delta T = 0.1$ the pseudogap is roughly the same as its value at lower temperatures, in the thermodynamic limit. In fact, for a temperature of $1.5T_c$ we find a pseudogap that is about 85% of its value as $\delta T \rightarrow 0$. So, the pseudogap energy does not change appreciably with temperature for small reduced temperatures (less than 0.1). At sufficiently high temperatures the pseudogap disappears, but we find that it does so by the DOS filling in, as opposed to the pseudogap energy going to zero.

As to whether or not the pseudogap persists for lower couplings, we have completed a similar analysis for $|U|/t = 3$ at half filling, and again find evidence for a pseudogap – the

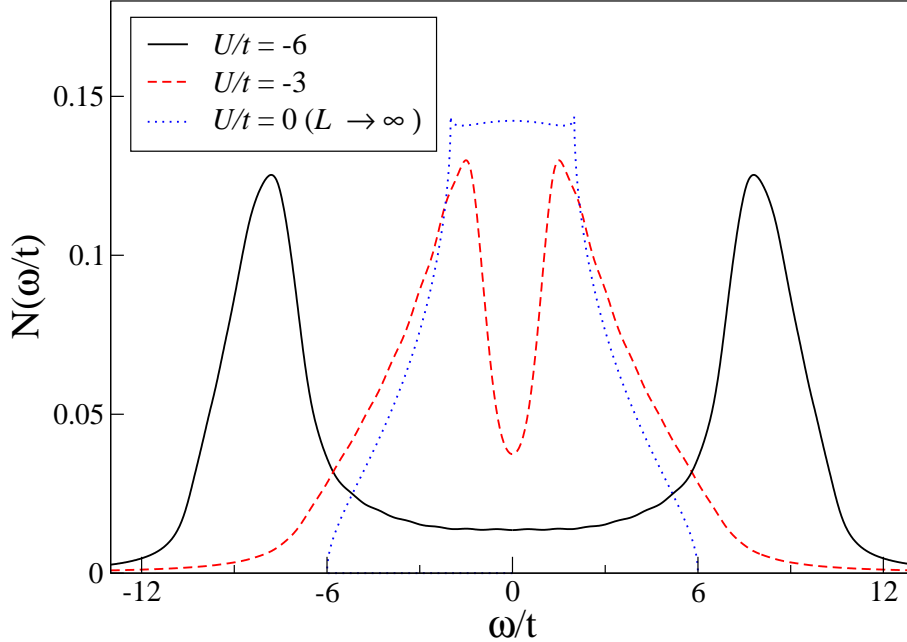


FIG. 7: DOS for $|U|/t = 6$ and 3 at half filling, for a 12^3 simple cubic lattice, at a temperature of $T = 1.001 T_c$. In this plot we have used the same broadening ($0.36t$) for both $U \neq 0$ curves. As a reference curve we also show the DOS of the noninteracting system in the thermodynamic limit.

analogue of Fig. 8 is shown in Fig. 9.⁶¹ We find the striking result that the extrapolated gap for smaller reduced temperatures is within 5% of the BCS gap! We emphasize that this matching of energy “gaps” is found between a $T = 0$ BCS gap and a $T_c < T_{\sim} < 1.001T_c$ pseudogap.

Our result, that is the existence of a pseudogap in a model of a three-dimensional strongly correlated electronic system, agrees with the earlier (three-dimensional) work of Levin *et al.*²⁸ However, they propose that the pseudogap they find can be understood in terms of a T-matrix resonance caused by intermediate to large U , whereas we are finding the full value of the BCS gap above T_c even for weak coupling.

For smaller reduced temperatures and large lattices our partial fractions algorithm fails, due to the high accuracy that must be enforced to find converged pole locations and residues. To be specific, we were unable to find a converged partial fractions decomposition even after 30 days of computation for $L = 12$ for reduced temperatures less than 0.0005.

Clearly, a thorough search of parameter space, that is for other electronic densities and for other ratios of $|U|/t$, is called for. Unfortunately, as mentioned earlier, it takes roughly 10

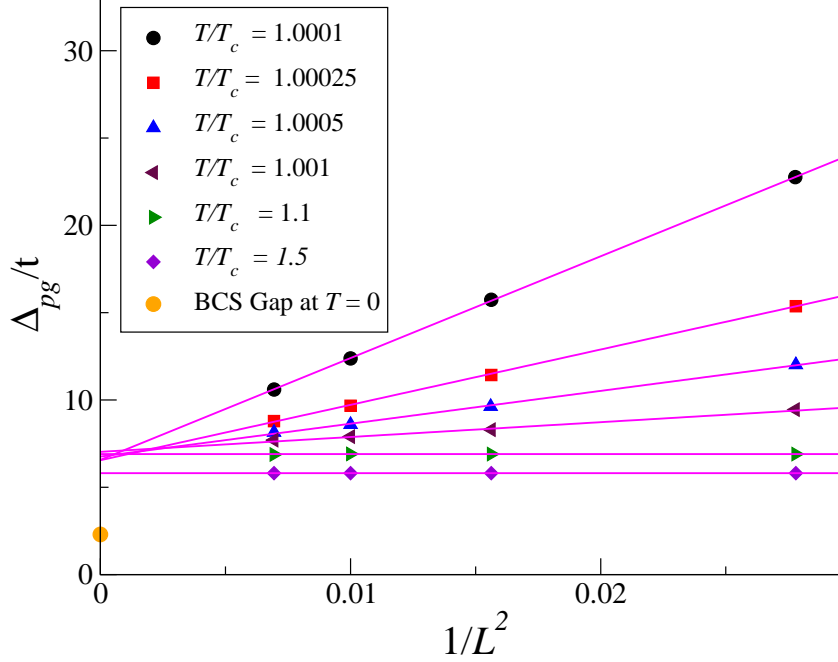


FIG. 8: The peak locations of the DOS, labelled as Δ_{pg} and expressed in units of t , for 3d simple cubic lattices of size 6^3 , 8^3 , 10^3 , and 12^3 , for $|U|/t = 6$ and $1/2$ filling, plotted as a function of one over the the system's linear size (L) squared, for a variety of temperatures (shown in the legend) just above the superconducting transition temperature. The solid lines are least squares fits for each temperature. The $T = 0$ superconducting gap (in the thermodynamic limit), found from the solution of the BCS gap equation, is also shown.

days to get each data point for a 12^3 lattice (for one temperature and one chemical potential), so new implementations of this approach are being explored in the hope of finding a more expedient algorithm.

V. CONCLUSIONS:

We have introduced a technique that allows for the extraction of the *real-axis dynamical properties* of the pair susceptibility, the self energy, and the spectral functions, for a strongly correlated electronic system when unrenormalized propagators are used. We have applied this technique to the attractive Hubbard model, and examined the properties of the density

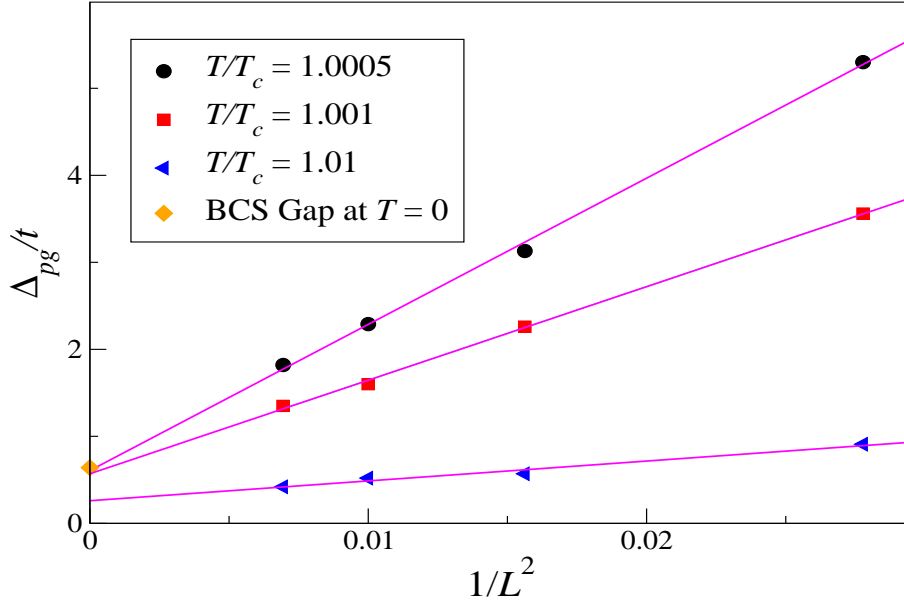


FIG. 9: The same quantities as in Fig. 8 are plotted for $|U|/t = 3$. Note that the extrapolated values of the pseudogap, at temperatures just above the superconducting transition temperature, are within 5% of the $T = 0$ BCS gap.

of states in the thermodynamic limit. Of particular interest for us is three dimensions, since a true transition at a nonzero temperature to a superconducting phase should be present for this model of correlated electrons, and for weak coupling, described quite well by the non self-consistent T-matrix approximation. We find a pseudogap in three dimensions that persists in the weak coupling limit, and whose energy is comparable to the $T = 0$ BCS gap energy in the same weak coupling limit; for larger $|U|/t$ we find a pseudogap energy that is much larger than the $T = 0$ BCS gap energy .

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